LQCD Project 2009 Annual Review

Overview and Collaboration Management

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For the USQCD Collaboration

http://www.usqcd.org

LQCD Project 2009 Annual Review
Fermilab
June 4-5, 2009

Synopsis

- Final annual review of the LQCD lattice computing hardware project, 2006-2009.
  - Hardware is located at BNL, JLab, Fermilab.
  - Project is funded jointly by DoE's offices of HEP and NP.

Year	FY2006	FY2007	FY2008	FY2009	Total
Hardware	$1,850	$1,592	$1,630	$798	$5,870
Operations	$650	$908	$870	$902	$3,330
Total	$2,500	$2,500	$2,500	$1,700	$9,200

Funding of the LQCD Computing Project in thousands of dollars.

- The LQCD Project is one of several hardware and software efforts overseen by the USQCD Collaboration.
- USQCD is a collaboration consisting of most US lattice gauge theorists. Its purpose is to develop the software and hardware infrastructure required for lattice gauge theory calculations.

Plan of talks

(Detailed schedule at http://projects.fnal.gov/lqcd/reviews/June2009Review/agenda.shtml .)

09:00 - Logistics and Introductions (10 min) - *Bill Boroski*

09:10 - Welcome (10 min) - *Vicky White*

09:20 - Project Overview (45 min) - *Paul Mackenzie*

10:05 – Fundamental Parameters of the Standard Model (40 min) - *Andreas Kronfeld*

10:45 - Break

11:00 - Hadron Spectroscopy, Structure and Interactions (40 min) - *John Negele*

11:40 - High Temperature/Density QCD (40 min) - *Frithjof Karsch*

12:20 - Lunch

1:00 - Beyond the Standard Model Physics (40 min) – *Simon Catterall*

1:40 - Project Management and Performance (60 min) - *Bill Boroski*

2:40 - Break

2:55 - Technical Design and Proposed Technical Scope for FY2009 (40 min) - *Don Holmgren*

3:35 - Responses to Scientific Recommendations from the 2008 Review (30 min) - *Paul Mackenzie*

4:05 - Responses to Technical Recommendations from the 2008 Review (20 min) - *Bill Boroski*

4:25 - Executive Session

5:30 - Committee request for additional information - *Committee/Project Leadership*

6:00 - Adjourn

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Plan of this talk

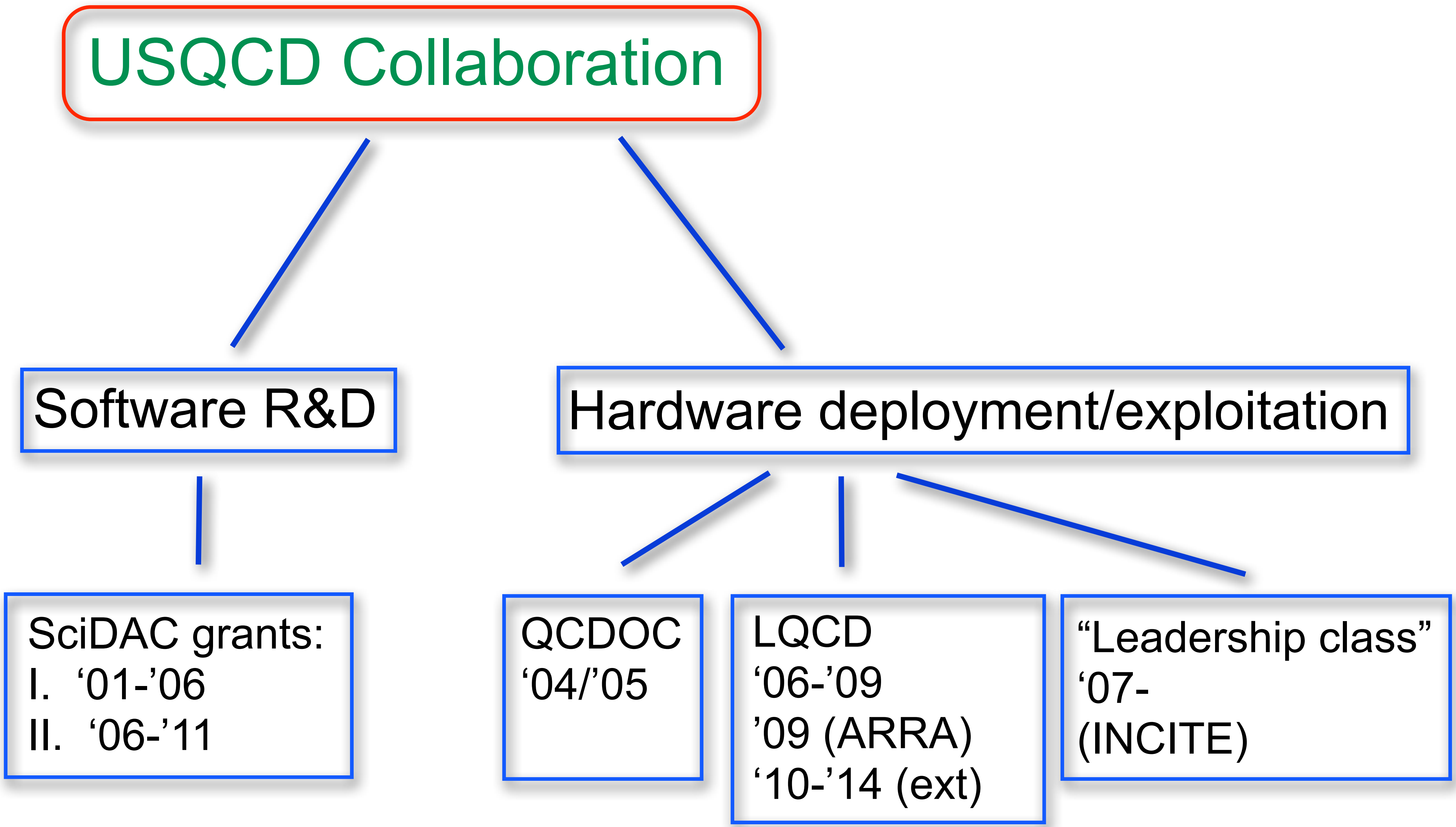
- The USQCD Collaboration
- Lattice QCD
- USQCD scientific goals.

I. The USQCD Collaboration

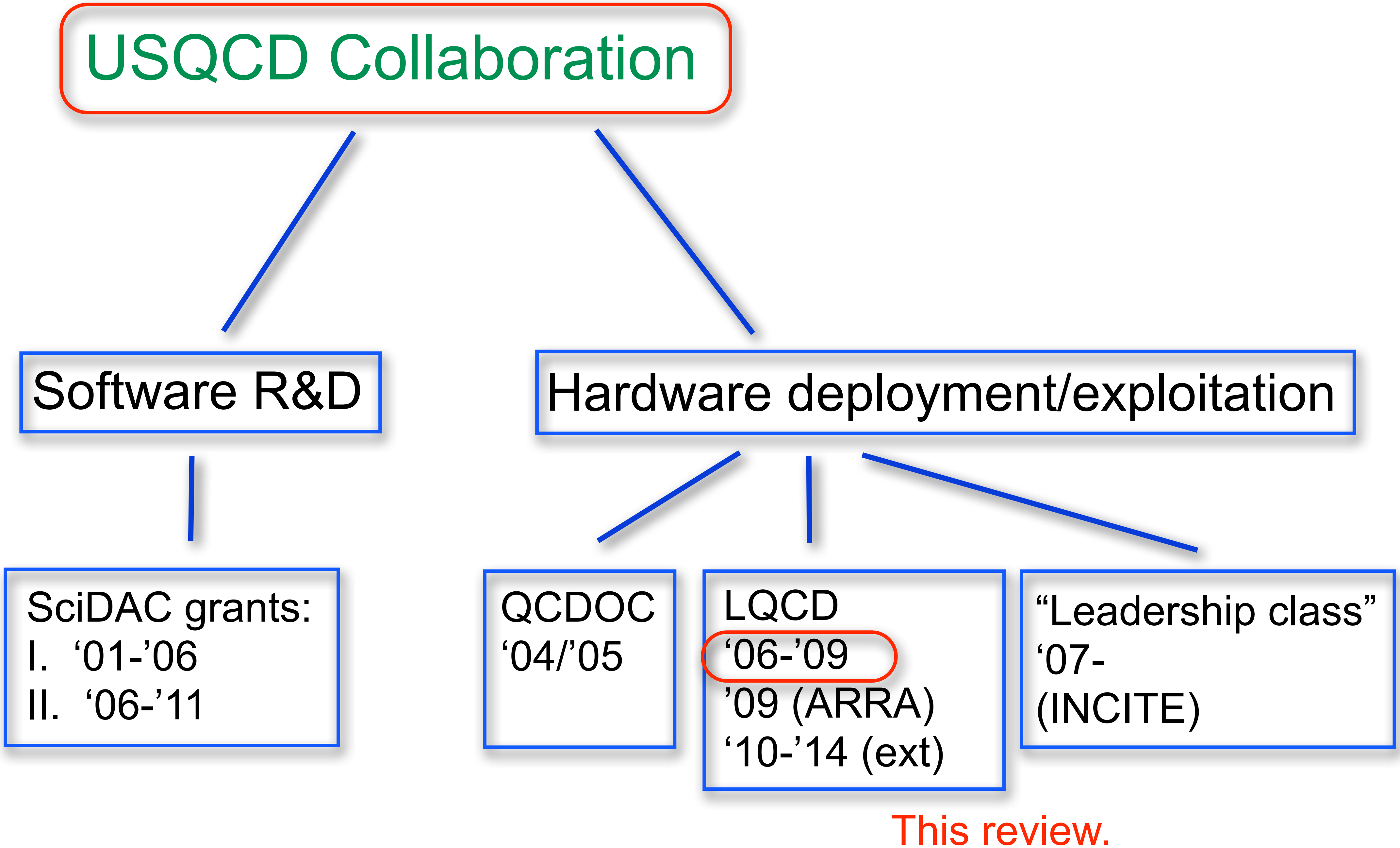
Because of the great potential for lattice calculations to advance the goals of the HEP and NP experimental programs, DoE asked the US lattice gauge theory community to organize itself to create software and hardware infrastructure for lattice calculations.

The USQCD Collaboration was the result.

Consists of the great majority of US lattice gauge theorists, ~145 members.
Purpose: develop hardware and software infrastructure for the US lattice community. (Physics projects are done by individual groups within USQCD.)



USQCD has grants for
- R&D for software development through the SciDAC program.
- Hardware deployment from several sources, including the current LQCD project.



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USQCD Collaboration

LQCD Hardware Project

Federal project manager: John Kogut (HEP)
Federal project monitor: Ted Barnes (NP)

Executive committee:
Paul Mackenzie (chair), Rich Brower, Norman Christ, Mike Creutz, John Negele, Claudio Rebbi, David Richards, Steve Sharpe, Bob Sugar

Contract project manager: Bill Boroski
Assistant project manager: Bakul Banerjee

Change control board: Paul Mackenzie (chair), Bill Boroski, Steve Gottlieb, Tom Schlagel, Vicky White, Roy Whitney

Scientific program committee:
Frithjof Karsch (chair)

Software committee:
Rich Brower (chair)

Project being reviewed today.

The USQCD collaboration is funded through SciDAC, through the LQCD project, and through base HEP and NP funds at BNL, Fermilab, and JLab.

USQCD collaboration web page: http://www.usqcd.org

USQCD hardware resources

	Machine	Location	2009/10 allocation (M 6n node-hours)	Subtotal	Total
LQCD hardware. Clusters.					
	Pion	Fermilab	2.55		
	6n	JLab	1.84		
	Kaon	Fermilab	7.59		
	7n	JLab	8.84		
	JPsi	Fermilab	24.9	45.72	
Other USQCD hardware resources					
	QCDOC	BNL	10.8	10.8	
	Incite BG/P	Argonne	18.1		
	Incite XT5	Oak Ridge	11.6	29.7	86.22
	Incite discretionary time ...				

1 M 6n node-hours
= 0.3 QCD TF-years
(where TF measured by real QCD production code), and
= ~ 1.5 Linpack TF-years
(where TF measured with Linpack).

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= ~ 1.5 Linpack TF-years
(where TF measured with Linpack).

Installed 08/09.
Holmgren talk.

SciDAC lattice QCD computing R&D

Software Committee:
Richard Brower (chair), Boston University, Carleton DeTar, University of Utah, Robert Edwards, JLab, Rob Fowler, UNC, Donald Holmgren, Fermilab, Robert Mawhinney, Columbia University, Pavlos Vranas, Lawrence Livermore Lab, Chip Watson, JLab

USQCD has a SciDAC-2 grant of ~$2.2M/year for creating lattice QCD software infrastructure: community libraries, community codes, optimization and porting to new architectures, implementation of up-to-the-minute algorithm advances...
This has enabled optimally efficient operation on the USQCD hardware.

Regular Thursday phone conferences for people working on USQCD software.

Software achievements

- The QCD API and community libraries
    - Lower entrance barriers to lattice QCD.
    - Enable postdocs to run major projects without being part of major collaborations.
- Porting and optimizations for new platforms
    - In 2008, USQCD was the only project with a multiyear program ready to run on the Argonne BG/P from the start. Used ~1/3 of cycles in 2008, accomplished a three-year program of configuration generation in one year.
- Projects in workflow, visualization, performance analysis, cluster reliability, ...

Incite resources

- The DOE allocates time on its leadership class supercomputers, the Cray XT4/XT5 at ORNL and the BlueGene/P at ANL, through its Incite Program.
  - These are highly suited to handling our largest computing jobs, especially generation of large gauge configuration ensembles.
- USQCD currently has a three year grant running from calendar year 2008 though calendar year 2010.
- Resources are allocated one year at a time. The USQCD allocation for 2009 is the largest in the program. It consists of:
  - 67 M core-hours on the BlueGene/P.
  - 20 M core-hours on the Cray XT4/XT5.

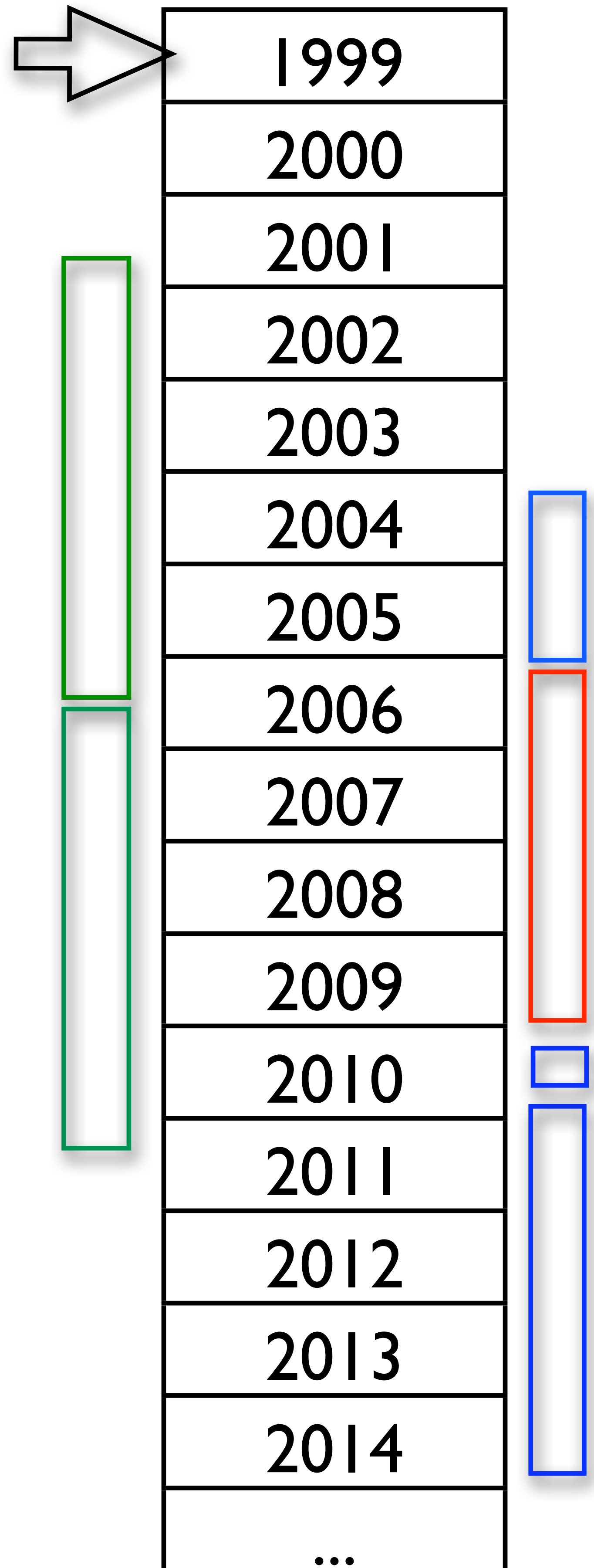
USQCD timeline

USQCD Executive Committee formed.

Software grants

First five-year SciDAC grant for lattice computing R&D.

Second five-year SciDAC grant for R&D.



Hardware grants

Construction of the QCDOC.

First cycle of continuous HEP and NP funding for hardware through LQCD project (this review).

Proposed ARRA computer.

Proposed LQCD-ext hardware project in 2010-2014.

Scientific Program Committee

Scientific Program Committee:
Frithjof Karsch (chair), BNL, Thomas Blum, U Conn., Christopher Dawson, Virginia, Robert Edwards, JLab, Andreas Kronfeld, Fermilab, Martin Savage, U. Washington, Junko Shigemitsu, Ohio

Each year, the many smaller physics collaborations within USQCD submit proposals to the Scientific Program Committee for allocations of time on USQCD's LQCD and Incite resources.

The SPC creates a program to accomplish the goals set forth in the computing proposals.

The Executive Committee seeks the advice of the SPC on physics priorities when writing new proposals for DoE computing resources.

Chair rotates every two years. Members rotate every three years. Current committee contains none of the original members.

Allocation process

- Each year, the SPC issues a call for proposals for use of LQCD resources and DoE leadership class (Incite) resources.
- Three types of proposals.
  - Type A. Large projects expected to benefit the whole collaboration by producing data, such as gauge configurations, for general use, or by producing physics results listed among USQCD's strategic goals.
  - Type B. Need not share data or work toward USQCD's goals (although if they do, it's a plus). Was under 0.5 M hours -> 1 M hours. Goal is 10-15% of total allocation. Currently undersubscribed.
  - Type C. Exploratory calculations such as for developing or benchmarking code.
- The SPC reviews proposals, then organizes an all-hands meeting of USQCD. Plans of proposals are discussed by their proponents and by the collaboration as a whole.

2009 USQCD all-hands meeting

- Took place May 14-15 at Fermilab. 62 members attended.
- Reports from the Executive Committee, the LQCD Assistant Project Manager (Bakul Banerjee), the SPC, the Software Committee, and the site managers.
- Round table discussions with
  - The SPC on the allocation process,
  - The Software Committee.
- Report from nuclear physicist Curtis Meyer on the nuclear physics Lattice QCD Meets Experiment meeting at JLab.

Outcome of the allocation process

- The fifteen Type A proposals were awarded 140.5 M 6n equivalent node-hours on LQCD and leadership class resources, 67.7% of amount requested.
- The sixteen Type B proposals were awarded 5.3 M 6n hours on LQCD resources, 119% of requested.
- 52% of the cycles were on leadership class computers, remaining 48% on LQCD Project computers.

Lattice QCD meets experiment meetings

To increase the interaction between lattice gauge theory and experiment, members of USQCD have organized a series of workshops with experimenters and phenomenologists.

- SLAC, Sept. 16, 2006, Standard Model physics. Co-organized with BaBar.
- Fermilab, December 10-11, 2007, Standard Model physics.
- Livermore, May 2-3, 2008, “Lattice Gauge Theory for LHC Physics”, Beyond the Standard Model physics.
    - No experimenters yet, but some BSM phenomenologists
- JLab, Nov. 21-22, 2008, “Revealing the Structure of Hadrons”, Nuclear physics.
- BNL, June 8-9, 2009, “Critical Point and Onset of Deconfinement”, QCD thermodynamics.

Starting in 2009, a member of the experimental community at each meeting will be invited to address the All-hands Meeting to assess the interaction between lattice and experiment at the meeting.

International collaboration

- Lattice QCD is an international field with very strong programs in Germany, Italy, Japan and the United Kingdom, and elsewhere. Groups within USQCD have formed a number of international collaborations:
  - The USQCD effort using DWF quarks is an international effort between the United States based RBC and LHPC Collaborations, and Edinburgh, Southampton and Swansea members of the UKQCD Collaboration.
  - The Fermilab Lattice, HPQCD and MILC Collaborations have worked together in various combinations to study heavy quark physics using improved staggered quarks. HPQCD includes physicists in both USQCD and UKQCD.
  - Members of the RBC Collaboration studying QCD thermodynamics using the P4 staggered quark action have a long term collaboration with physicists at the University of Bielefeld, Germany.
  - Members of USQCD working on the hadron spectrum using Clover quarks on anisotropic lattices have close ties with colleagues in Trinity College, Dublin.

International cooperation

- USQCD has played an active role in the formation and work of the International Lattice Data Grid (ILDG) which is organizing the sharing of large data sets (gauge configurations and quark propagators) on the international level.
- The ILDG has developed standards for file format and content, and the middleware needed to archive and retrieve files.
- Groups in Europe, Japan and the United Kingdom, as well as those in the United States, are all making data sets available through the ILDG.

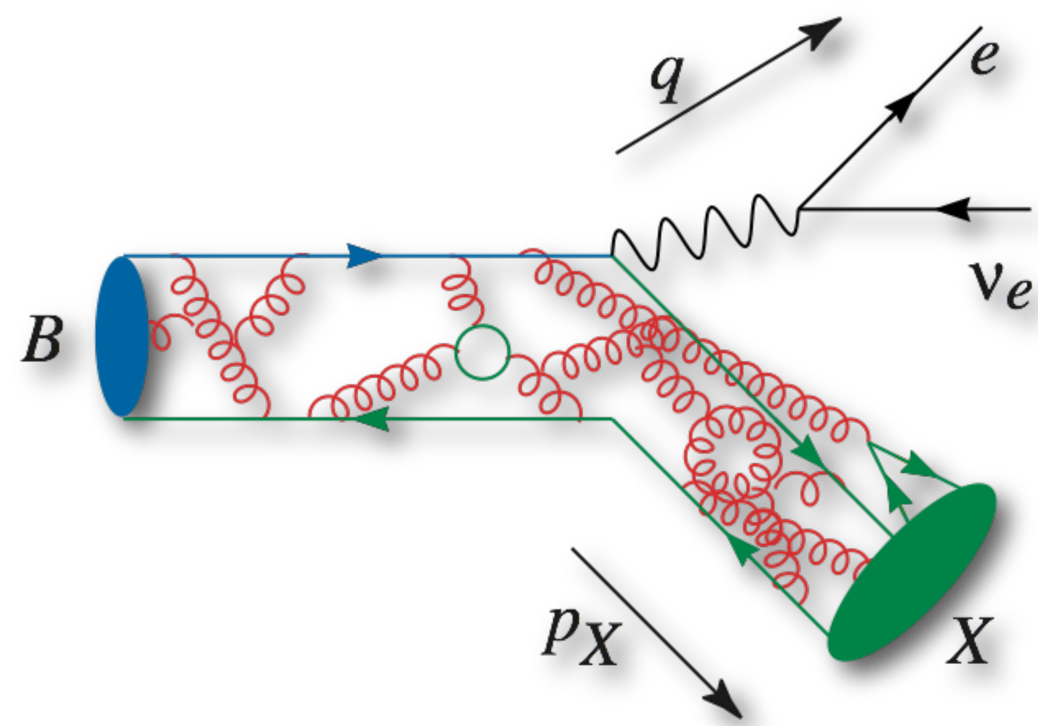
II. Lattice QCD

QCD is the theory of quarks and gluons. Quarks and gluons cannot be directly observed because the forces of QCD are strongly interacting.

Quarks are permanently confined inside hadrons, even though they behave as almost free particles at asymptotically high energies.

"Asymptotic freedom", Gross, Politzer, and Wilczek, Nobel Prize, 2004.

Lattice QCD is used to relate the observed properties of hadrons from the properties of their quark and gluon constituents.



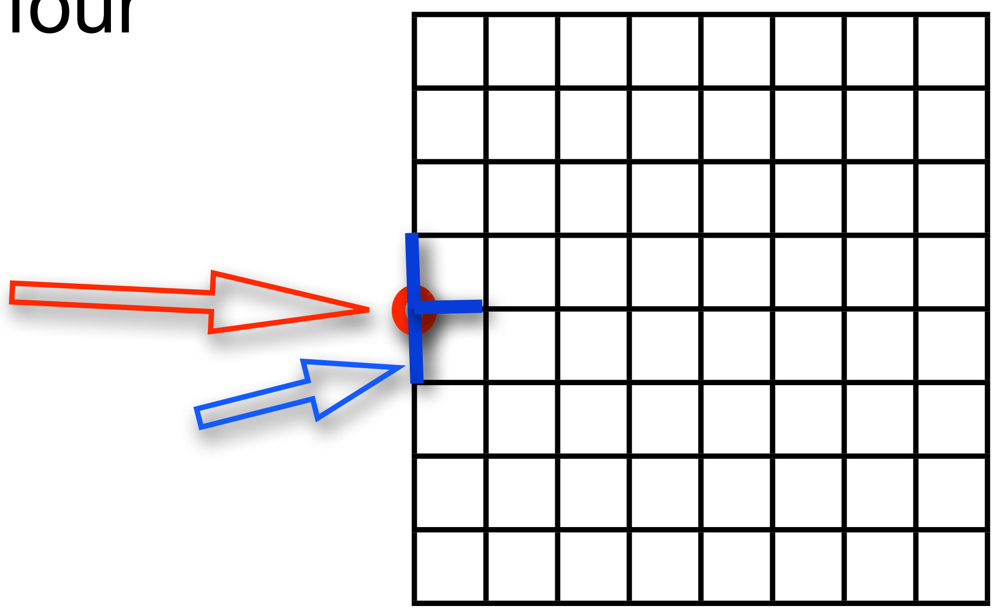
$B \to \pi l \nu$ semileptonic decay

Luke

Lattice quantum field theories

Approximate the path integral of quantum field theory by defining the fields on a four dimensional space-time lattice.

Quarks (ψ) are defined on the sites of the lattice, and gluons (U_μ) on the links.



Monte Carlo methods are used to generate a representative ensemble of gauge fields. Relaxation methods are used to calculate the propagation of quarks through the gauge field.

Continuum quantum field theory is obtained in the zero lattice spacing limit. This limit is computationally very expensive.

The Dirac, or “Dslash”, operator

The fundamental operation that consumes the bulk of our cycles is the solution of the Dirac equation on the lattice.

The fundamental component of the Dirac operator is the discrete difference approximation to the first derivative of the quark field on the lattice.

$$\partial_\mu \psi(x) \rightarrow \Delta_\mu \psi(x) \approx \frac{1}{2a}(\psi(x+\hat{\mu}a) - \psi(x-\hat{\mu}a)) + \mathcal{O}(a^2)$$

Quarks in QCD come in three colors and four spins.
The color covariant Dslash operator of lattice QCD is

$$D_\mu \gamma_\mu \psi(x) \equiv \frac{1}{2}\left(U_\mu(x)\gamma_\mu \psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\gamma_\mu \psi(x-\hat{\mu})\right)$$

γ operates on spin four-vector.

U operates on color three-vector of the quark.

The bulk of the $O(10^{22})$ flops envisioned in this project are consumed in multiplying complex 3-vectors by 3x3 complex matrices.

Controlling systematic errors

- Finite lattice spacing errors: Calculations must be performed at several small values of the lattice spacing in order to extrapolate to the continuum limit.
- Chiral extrapolation errors: Calculations must be performed at several small values of the up and down quark masses to extrapolate to their physical values using chiral perturbation theory.
- Improved actions: The use of actions (improved formulations of QCD on the lattice) greatly increases the accuracy of these extrapolations,for reaching our scientific goals.

The computational challenge of lattice QCD

Lattice	Quark			Gauge	ensembles		Analysis propagators, correlators		
spacing *a* (fm)	**mass *ml/ms***	**Volume (sites)**	**Configu rations**	**Core-hours (M)**	**TB/ ensemble**	**Files/ ensemble**	**Core-hours (M)**	**TB/ ensemble**	**Files/ ensemble**
0.06	0.1	64^3*144	1000	32.36	10.9	1,000	32	696	155,000
	0.15	56^3*144	1000	14.04	7.3	1,000	14	466	“
	0.2	48^3*144	1000	6.74	4.6	1,000	7	294	“
	0.4	48^3*144	1000	3.66	4.6	1,000	4	294	“
0.09	0.1	40^3*96	1000	3.43	1.8	1,000	3	113	155,000
	0.15	28^3*96	1000	0.81	0.6	1,000	0.8	39	“
	0.2	28^3*96	1000	0.62	0.6	1,000	0.6	39	“
	0.4	28^3*96	1000	0.36	0.6	1,000	0.4	39	“
0.12	0.1	24^3*64	1000	0.38	0.3	1,000	0.4	16	155,000
	0.15	20^3*64	1000	0.15	0.1	1,000	0.2	9	“
	0.2	20^3*64	1000	0.12	0.1	1,000	0.1	9	“
	0.4	20^3*64	1000	0.07	0.1	1,000	0.1	9	“

Example gauge ensemble library.

CPU times normalized in BG/P core-hours.

Operationally, lattice QCD computations consist of

1) Sampling a representative set of gauge configurations with Monte Carlo methods,

   E.g., the Metropolis method, the hybrid Monte Carlo algorithm, ...
   Consists of one long Markov chain.

2) Calculating the propagation of quarks through the gauge configurations,

   Solve the Dirac equation on each configuration with relaxation methods, e.g., biconjugate gradient algorithm, etc

3) Constructing hadron correlation functions from the quark propagators (smaller task).

Anatomy of a typical lattice calculation

Near-TB file sizes

Generate gauge configurations on a leadership facility or supercomputer center.
Tens of millions of BG/P core-hours.

Transfer to labs for analysis on clusters. Comparable CPU requirements.

A single highly optimized program,
very long single tasks,
moderate I/O and data storage.

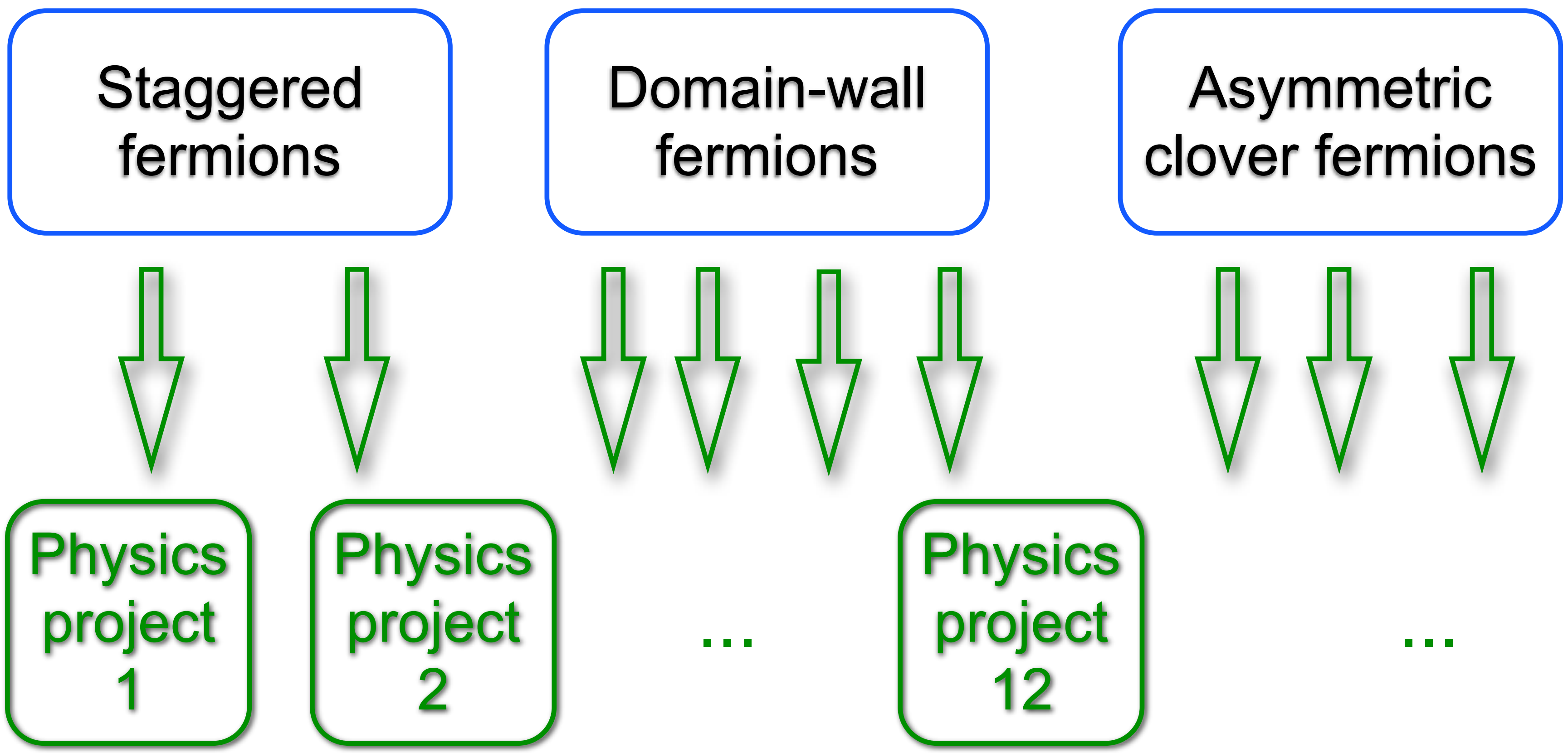
Large, heterogeneous analysis code base,
10,000s of small, highly parallel tasks,
heavy I/O and data storage.

Two comparably sized jobs with quite different hardware requirements.

US lattice gauge theory sociology

Zero-temperature QCD:

Currently three main streams of QCD gauge configurations are being generated by USQCD:



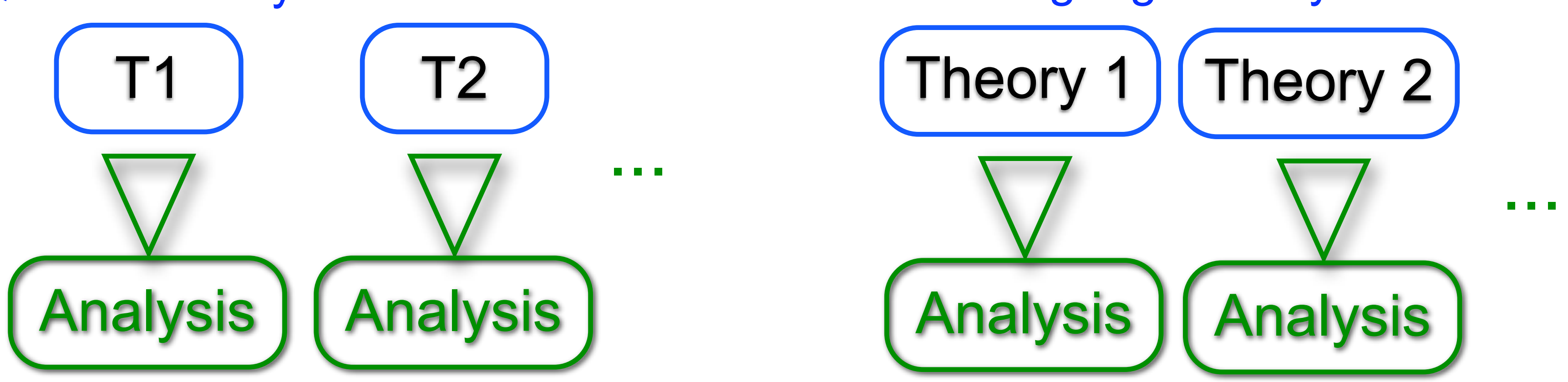
Shared among a couple of dozen groups, in both HEP and NP.

Physics projects are done on these configurations by smaller groups of 5-15 members within USQCD.

Around 90 of the 145 members of USQCD have submitted jobs to USQCD hardware.

QCD thermodynamics:

BSM gauge theory:



Purposes of ensembles

Currently three main streams of QCD gauge configurations are being generated by USQCD:

Staggered fermions	Domain-wall fermions	Asymmetric clover fermions
Tuned toward small lattice spacings and light quark masses for precision on Standard Model parameters.	Tuned toward larger volumes for accurate nucleons and two-pion states.	Tuned toward very small lattice spacings in time for investigation of excited states.
$a \sim 0.045 - 0.18$ fm, $m_l > 0.05\ m_s$, V~(2.4 fm)^3.	$a \sim 0.081 - 0.114$ fm, $m_l > 0.12\ m_s$, V ~ (2.7 fm)^3.	$a_s \sim 0.122$ fm, $a_t \sim 0.035$ fm, $m_l \to 0.037\ m_s$ (=m_{phys}) V $\to$ (5 fm)^3.
Next: asqtad $\to$ hisq.	Next: $\to$ AuxDet.	

2008 USQCD physics projects

Yasumichi Aoki	Proton Decay Matrix Elements
Christopher Aubin	Delta Moments Using Background Field Techniques
Tom Blum	Electromagnetic Effects in Hadrons
Rich Brower	QCD Vacuum Polarization Contribution to the S Parameter and g-2
Simon Catterall	Supersymmetry and Strong Dynamics on the Lattice
Norman Christ	Simulations with Dynamical Domain Wall Fermions
Carleton DeTar	Quarkonium Physics with Unquenched Improved Staggered Fermions
Jozef Dudek	Spectral and Radiative Meson Physics of GlueX and CLEO-c
Robert Edwards	Dynamical Anisotropic-Clover Lattice Production for Hadronic Physics
George Fleming	Strong LHC Physics on the Lattice
James Hetrick	π-π Scattering with Staggered Quarks and All-to-All Propagators
Jimmy Juge	Simulating Two-Particle States on Dynamical, Anisotropic Lattices
Julius Kuti	Nonperturbative Higgs Physics
Jack Laiho	B_K with Domain-Wall Valence Quarks and 2+1 Staggered Sea Quarks
Peter Lepage	High-Precision Heavy-Quark Physics
Huey-Wen Lin	Study of Excited Form Factors Using Dynamical Anisotropic Lattice
Keh-Fei Liu	Nucleon Form Factors and Hadron Spectroscopy
Paul Mackenzie	*B* and *D* Meson Decays with Unquenched Improved Staggered Fermions
Robert Mawhinney	B_K, f_π, f_K, and Quark Masses from 2+1 Flavor DWF Lattices
Harvey Meyer	Shear and Bulk Viscosity of SU(3) Yang-Mills Theory
John Negele	Nucleon Structure in the Chiral Regime with Domain Wall Fermions
Ethan Neil	Lattice Study of Nf = 10 Yang-Mills Theory
Kostas Orginos	Octet Baryon Form Factors
James Osborn	Strange Quark Contribution to Nucleon Form Factors
Peter Petreczky	QCD Thermodynamics with Improved Staggered Fermions: Towards the Physical Quark Mass
David Richards	Baryon Spectroscopy using Anisotropic Clover Lattices
Martin Savage	Lattice QCD for Nuclear Physics
Stephen Sharpe (1)	B_K and Related Matrix Elements with Unquenched, Improved Staggered Fermions
Stephen Sharpe (2)	Non-perturbative Renormalization with Improved Staggered Fermions
Robert Sugar	QCD with Three Flavors of Improved Staggered Quarks
Andre Walker-Loud	Hadronic Electromagnetic Properties
Walter Wilcox	External Field Simulations Using Dynamical Clover Fermions

2008 USQCD physics projects

Projects for configuration generation

Projects by post-docs

Beyond-the-Standard-Model projects

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David Richards	Baryon Spectroscopy using Anisotropic Clover Lattices
Martin Savage	Lattice QCD for Nuclear Physics
Stephen Sharpe (1)	B_K and Related Matrix Elements with Unquenched, Improved Staggered Fermions
Stephen Sharpe (2)	Non-perturbative Renormalization with Improved Staggered Fermions
Robert Sugar	QCD with Three Flavors of Improved Staggered Quarks
Andre Walker-Loud	Hadronic Electromagnetic Properties
Walter Wilcox	External Field Simulations Using Dynamical Clover Fermions

Main scientific thrusts

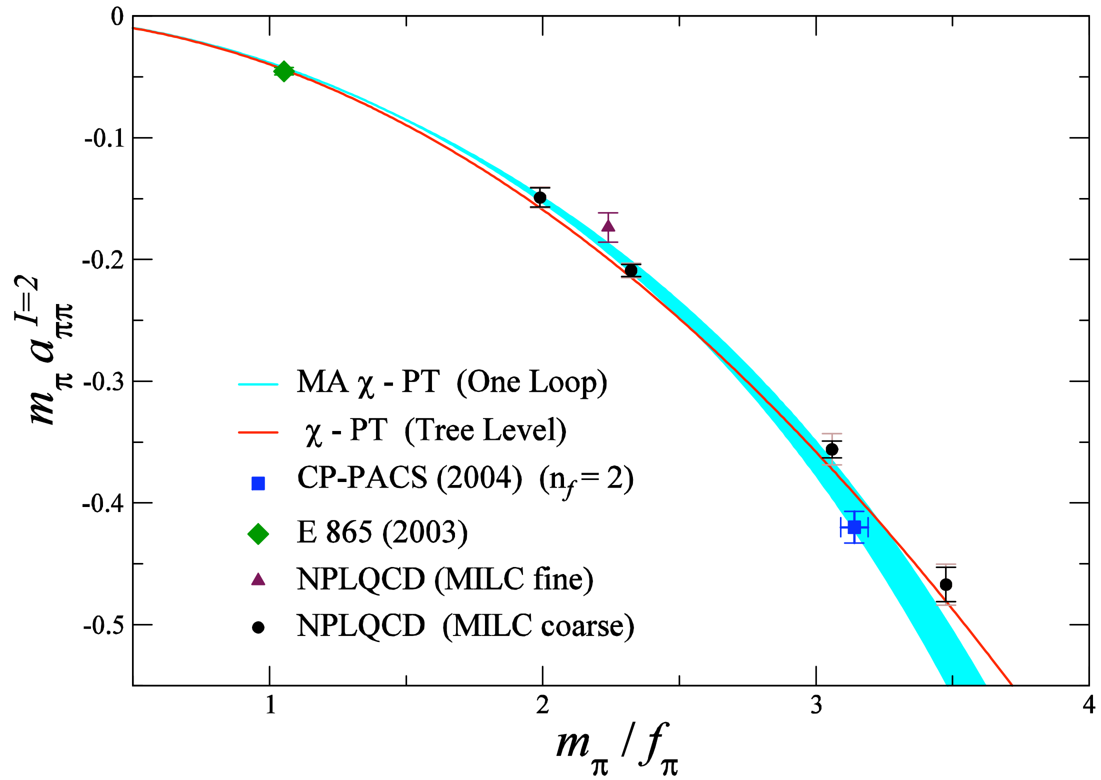
- Determining the fundamental parameters of the Standard Model from hadron physics. Talk by Andreas Kronfeld.
  - Experiments impacted: BaBar (SLAC), Belle (KEK), CLEO-c (Cornell), CDF and D0 (FNAL) and LHC (CERN).
- Understanding the structure and interactions of nucleons. Talk by John Negele.
  - Experiments impacted: CEBAF (JLab), RHIC (BNL).
- Understanding the behavior of QCD in extreme conditions. Talk by Frithjof Karsch.
  - Experiments impacted: RHIC (BNL), FAIR (GSI) and LHC (CERN).
- Understanding the properties of new strongly interacting gauge theories that may be discovered at the LHC. Talk by Simon Catterall.
  - Experiments impacted: LHC (CERN)?

Examples of results

- Hadron-hadron interactions

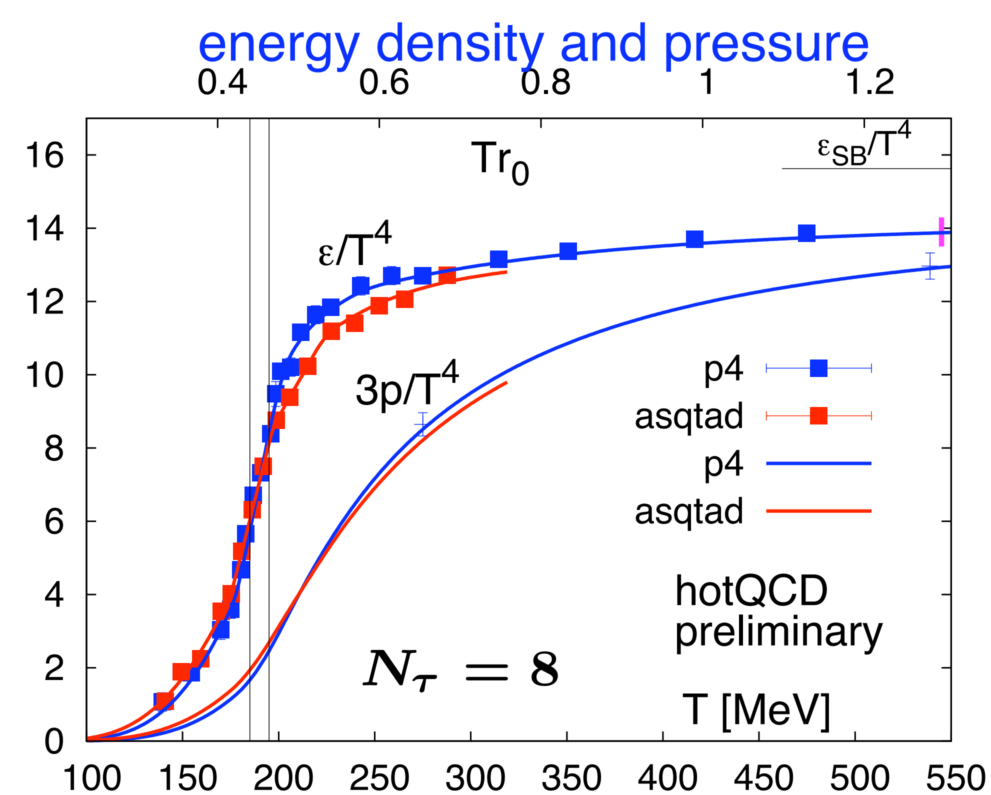
First 2+1 fully dynamical calculations of *ππ*, *πK*, and *KK* scattering lengths.

NPLQCD
Phys. Rev. D77:014505 (2008).
Phys. Rev. D73:054503 (2006).



- QCD in extreme conditions

RIKEN-BNL-Columbia-Bielefeld,
Phys. Rev. D77, 014511 (2008)
hotQCD collaboration.



Examples of results

- Beyond the Standard Model physics.

  No experiments to compare with yet, but we are preparing for the time when there will be.

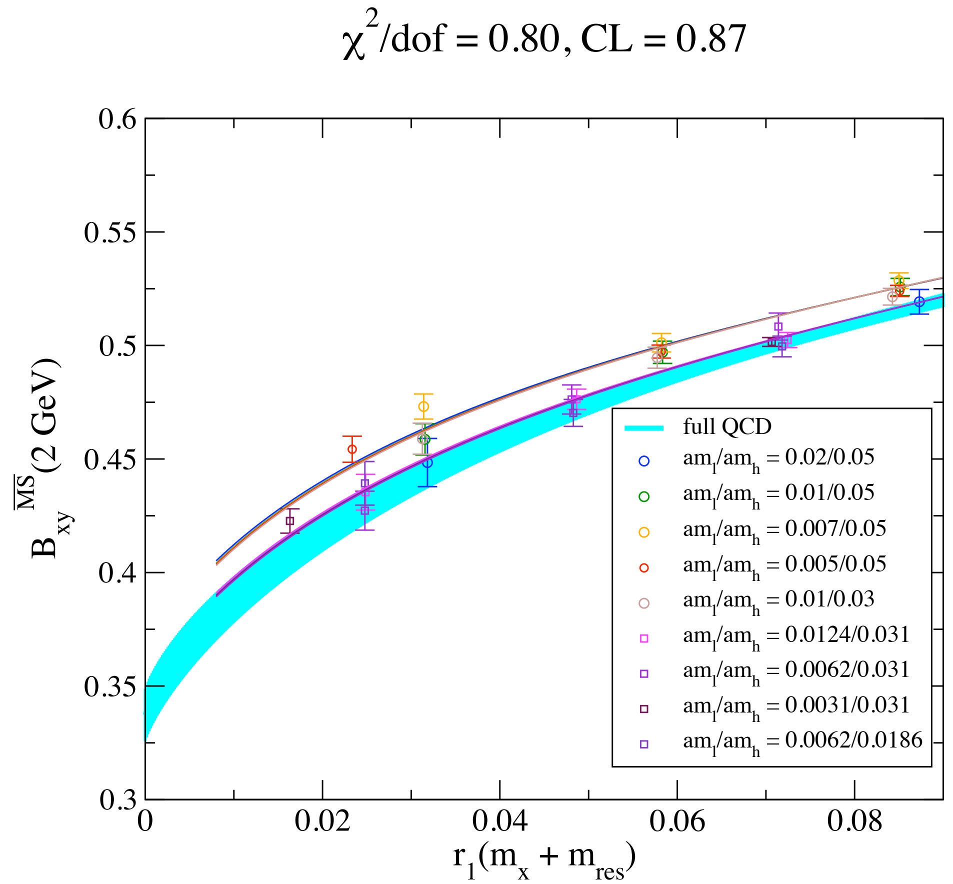
- Standard Model parameters.

  Kaon-antikaon mixing parameter B_K, constrains the CP violating parameters ρ and η.

  $$\widehat{B}_K = 0.724(8)(28).$$

  Three post-docs used USQCD resources to compete with much larger and well-established collaborations on an even footing.

  Aubin, Laiho, Van de Water. arXiv:0905.3947 [hep-lat].



The experimental mixing quantity here is already known to better than 1%.
Likewise for B mixing and Bs mixing.
Urgent to improve lattice calculations further to drive experiment forward!

The next four talks will cover these areas in detail.